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14. ABSTRACT A distributed dislocation method has been developed to quantify the elastic fields of inclusion eigenstrain problems in 2D and 3D (Lerma et al. 2003). The inclusions can be of any shape or size and the eigenstrains can be arbitrarily assigned, i.e. constant or non-constant within the inclusion. The method works well for material or field points inside or outside the inclusion domain, and is straightforward to apply. The method is based on discretizing the inclusion-matrix interface into a mesh of small regions of misfit represented in the method by dislocation loops with appropriately assigned Burgers vectors. The method works well for relatively far points from the inclusion although it also works for relatively close points at the expense of increasing the mesh density, i.e. the computational time involved. It was shown that, with increasing mesh density, the method converges onto known analytical solutions for some specialized geometry and misfits. Recently, we have developed a new distributed-dislocation method for modeling eigenstrain problems such as gamma prime inclusions/particles in nickel-base superalloys. Here the dislocation loops representing the misfit are distributed throughout the volume of the inclusion with the dislocation lines themselves lying on the inclusion-matrix interface. In addition we have performed 3D Dislocation Dynamics (DD) simulations to capture the strengthening effect of dilute misfit particle concentrations (Khraishi et al. 2003, 2004). The simulations were concerned with metal-matrix composites (MMCs) and focused on the strengthening effect associated with eigenstrain fields and not image stresses. These initial simulation results indicated a strengthening effect of one to three times higher than measured experimentally. This was done taking into account the effect of parameters such as particle radius, relative initial particle-dislocation source configuration, and number of particles. The simulations suggested that particle volume fraction is a strong indicator of the strengthening effect of particles in MMCs. In addition, simulations of the strengthening effect of low-angle grain boundaries were also performed and shed some light on interesting observations (Khraishi et al. 2003). Also, a study of a Bauschinger-like effect during cyclic loading was performed using 3D DD (Leger et al. 2004). Results indicated that, in some material systems, this effect could be explained by dislocation-particle interactions. Lastly, our 3D code has been now enhanced to handle in a rigorous way a larger variety of boundary conditions imposed on the simulation box's external surfaces. In particular, the emulation of free surface effects on the overall plasticity of these small simulation volumes can now be captured (Yan et al. 2003, 2004).				
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**FUNDAMENTAL STUDIES OF STRENGTHENING MECHANISMS IN METALS  
USING DISLOCATION DYNAMICS**

**AFOSR AWARD NO. F49620-01-1-0565**

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**Abstract**

A distributed dislocation method has been developed to quantify the elastic fields of inclusion eigenstrain problems in 2D and 3D (Lerma et al. 2003). The inclusions can be of any shape or size and the eigenstrains can be arbitrarily assigned, i.e. constant or non-constant within the inclusion. The method works well for material or field points inside or outside the inclusion domain, and is straightforward to apply. The method is based on discretizing the inclusion-matrix interface into a mesh of small regions of misfit represented in the method by dislocation loops with appropriately assigned Burgers vectors. The method works well for relatively far points from the inclusion although it also works for relatively close points at the expense of increasing the mesh density, i.e. the computational time involved. It was shown that, with increasing mesh density, the method converges onto known analytical solutions for some specialized geometry and misfits. Recently, we have developed a new distributed-dislocation method for modeling eigenstrain problems such as gamma prime inclusions/particles in nickel-base superalloys. Here the dislocation loops representing the misfit are distributed throughout the volume of the inclusion with the dislocation lines themselves lying on the inclusion-matrix interface.

In addition we have performed 3D Dislocation Dynamics (DD) simulations to capture the strengthening effect of dilute misfit particle concentrations (Khraishi et al. 2003, 2004). The simulations were concerned with metal-matrix composites (MMCs) and focused on the strengthening effect associated with eigenstrain fields and not image stresses. These initial simulation results indicated a strengthening effect of one to three times higher than measured experimentally. This was done taking into account the effect of parameters such as particle radius, relative initial particle-dislocation source configuration, and number of particles. The simulations suggested that particle volume fraction is a strong indicator of the strengthening effect of particles in MMCs.

In addition, simulations of the strengthening effect of low-angle grain boundaries were also performed and shed some light on interesting observations (Khraishi et al. 2003). Also, a study of a Bauschinger-like effect during cyclic loading was performed using 3D DD (Leger et al. 2004). Results indicated that, in some material systems, this effect could be explained by dislocation-particle interactions. Lastly, our 3D code has been now enhanced to handle in a rigorous way a larger variety of boundary conditions imposed on the simulation box's external surfaces. In particular, the emulation of free surface effects on the overall plasticity of these small simulation volumes can now be captured (Yan et al. 2003, 2004).

## Research Objective

The objective of this research effort is to develop fundamental understandings of some of the strengthening mechanisms that exist in crystalline metallic materials. This is accomplished via rigorous theoretical and numerical treatments, and comparisons with experiments where applicable. One aspect of this broader goal is to focus on misfit particles in a crystalline matrix and examine how their presence affects dislocation motion (i.e. plasticity-inducing elements in the metal). This is achieved by developing a generalized methodology in 2D and 3D to quantify misfit particles' stress and displacement fields. Such a generalization necessitates specific numerical schemes. Another objective is to utilize these misfit particle fields in a 3D Dislocation Dynamics (DD) framework and capture the micromechanics of dislocation-particle interaction. From the small-scale mechanics, DD also naturally allows for projection of results to a larger mesoscopic scale. The simulations in the second objective are sought for *both* monotonic and cyclic loading. A last objective is to use DD to investigate the strengthening effect offered by grain boundaries and the effect of free surfaces on the strength of the material.

## A Distributed-Dislocation Method for 2D Eigenstrain Problems

For inclusion problems Eshelby (1957) amongst others, introduced the eigenstrain method to quantify the elastic fields of these inclusions inside the inclusion and outside in the matrix. Such a method allows the derivation of analytical solutions of these problems (Mura 1982). Such solutions, however, are typically found for specialized inclusion geometry and simple eigenstrain expression (mostly for constant eigenstrain). This is so since finding analytical solutions for any arbitrary problem is almost impossible due to the complicated integration steps involved in this method. Moreover, the analytical method differentiates between the inclusion domain and the matrix domain in the solution procedure, with the elastic fields in the inclusion domain typically much easier to find.

Here, we have developed a numerical method to find the elastic fields of these inclusions for arbitrary situations. The method is based on two ideas: (1) An eigenstrain can be considered as a misfit between the inclusion and the matrix. (2) Any small misfit region can be modeled as a dislocation loop with appropriately assigned Burgers vector. The simplest eigenstrain problem is that of an elastic, infinitely long cylindrical bar inserted or fitted into a slightly smaller cylindrical hole in an infinite elastic medium. Here, the misfit region between the two is simply a cylindrical shell. To solve this problem, based on the above two ideas, the shell or misfit region is meshed such that each element represents a dislocation loop with some appropriately assigned Burgers vector. Figure 1 shows one of the meshes used for the case of an elliptical particle or inclusion. Figure 2 shows some plots of  $\sigma_{xy}$  along the  $x$ -axis inside the particle. The solid line is the analytical solution (Mura 1982). As seen in the figure, the plots from the numerical solution introduced above converged onto the analytical one as the number of mesh elements, or dislocation loops, increased. It is to be noted here that other geometry and eigenstrains have been investigated and the method worked for all of them.

## A Distributed-Dislocation Method for 3D Eigenstrain Problems

One can easily extend the above method for 2D misfit particle problems to treat 3D problems. The simplest case to consider here is that of a spherical particle fitted into a smaller spherical cavity. The ensuing elastic fields for the case of constant normal eigenstrains inside the particle have been given analytically by Teodosiu (1982). For the case of *shear* eigenstrain, the solution is given in Mura (1982). This latter solution is compared against our numerical solution in Figure 3. As seen again here, the numerical solution converges onto the analytical one for larger mesh densities. Here again different eigenstrains have been tried and the numerical method worked for all of them.

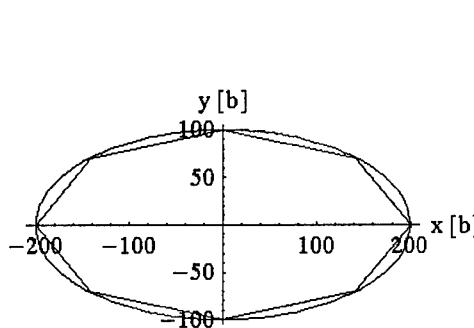


Figure 1: The mesh used in discretizing the misfit region around an elliptical inclusion.

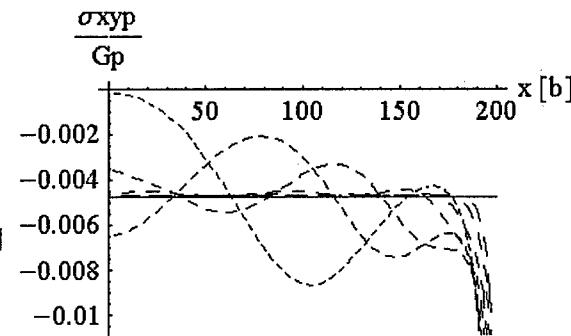


Figure 2: Normalized  $\sigma_{xy}$  stress inside the elliptical particle along the  $x$ -axis for increasing number of loops. This is for the case of constant *shear* eigenstrains inside the particle.

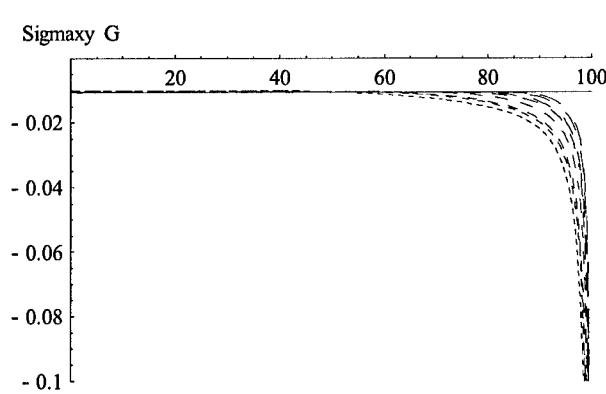


Figure 3: A plot of  $\sigma_{xy}/G$  along the  $x$ -axis inside a particle of 100 units in radius. The different dash sizes correspond to different mesh densities (larger dashes are for denser meshes).

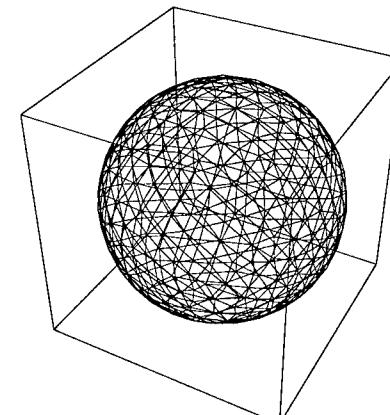


Figure 4: 3D triangular surface mesh of a spherical particle.

## Dislocation Dynamics (DD) Simulations of Particle Strengthening in MMCs

In this part of our research, we have investigated the strengthening effect of particles embedded in a metal-matrix, i.e. metal-matrix composites or MMCs. In particular, we have focused our investigation on dilute particle concentrations. In such systems, the likelihood of a dislocation-particle head-on collision is minute and therefore most strengthening in the composite would come from the eigenstrain field associated with the embedded particles (i.e. thermally-induced stresses).

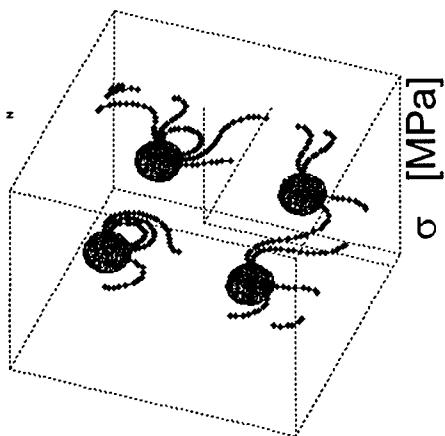


Figure 5: A snapshot of the simulations illustrating dislocation storage, in the form of glide dislocation pile-ups, in the dislocation source's glide plane above four particles.

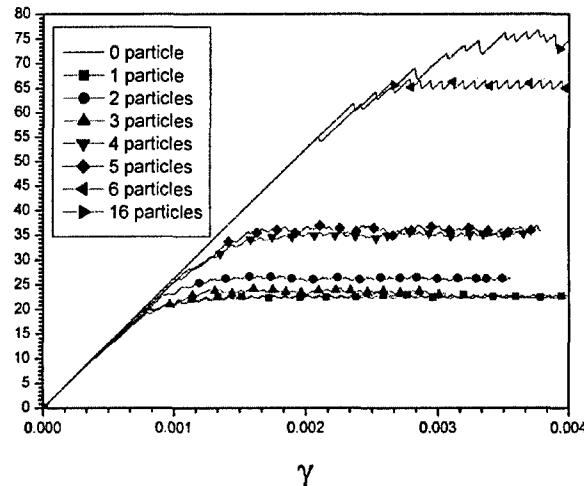


Figure 6: Simulated stress ( $\sigma_{yz}$ ) versus shear strain ( $\gamma_{yz}$ ) for different number of particles. This plot shows the effect of particle number, or volume fraction, on the flow stress value.

Here the matrix used in the simulations was aluminum and the particles were made of SiC. As the dislocations hovered over the particles, as in Figure 5, they were captured in the strain field of these particles in the form of pile-ups of glide dislocation loops. These pile-ups provided for an increase in the flow stress of the material as can be seen in Figure 6. The results indicated that particle volume fraction is a major parameter for measuring the expected strengthening due to particles in these composites.

## A Distributed-Dislocation Method for 3D Eigenstrain Problems

For inclusion problems where a volume misfit is present (for example gamma prime particles in nickel-base superalloys), there are inherently three linear misfit directions that are perpendicular to one another. More generically these misfit problems are termed eigenstrain problems. Currently no analytical methods are capable of calculating the elastic fields, i.e. displacement, strain and stress, of these particles/inclusions especially if the particle shape is not a simple shape such as a sphere or a cube. For example, real gamma prime particles are of cuboidal, spheroidal or lamellar shapes. To handle all such different and general shapes numerical models are needed.

From dislocation theory each closed dislocation loop represents a planar misfit. If one distributes such planar misfits or dislocation loops along an axis in space one can then reproduce a volume misfit along that direction, i.e. an eigenstrain along that direction in space. The easiest dislocation loops to think about or imagine are prismatic dislocation loops where the Burgers vector or misfit is perpendicular to the loop habit plane. Distributing such loops along the  $x$ -axis would produce a normal  $\varepsilon_{xx}^*$  eigenstrain. This is shown schematically in Figure 7a. Note that the dislocation lines of these loops define the boundary of the particle, or the particle-matrix interface. One can also distribute loops along the  $y$ -axis, as in Figure 7b, to produce a normal  $\varepsilon_{yy}^*$  eigenstrain. Finally, one can distribute loops in all three orthogonal directions, Figure 7c, to produce normal  $\varepsilon_{xx}^*$ ,  $\varepsilon_{yy}^*$  and  $\varepsilon_{zz}^*$  eigenstrains simultaneously. In this method, the misfit in one direction is equal to the sum of the Burgers vectors along this direction. Also, the more loops distributed along a certain length or dimension  $L$ , for example along a cubic particle side, the smaller their Burgers vectors are going to be and the more convergent the numerical solution is toward the actual solution, i.e. the more the numerical problem will mimic the real situation in a material.

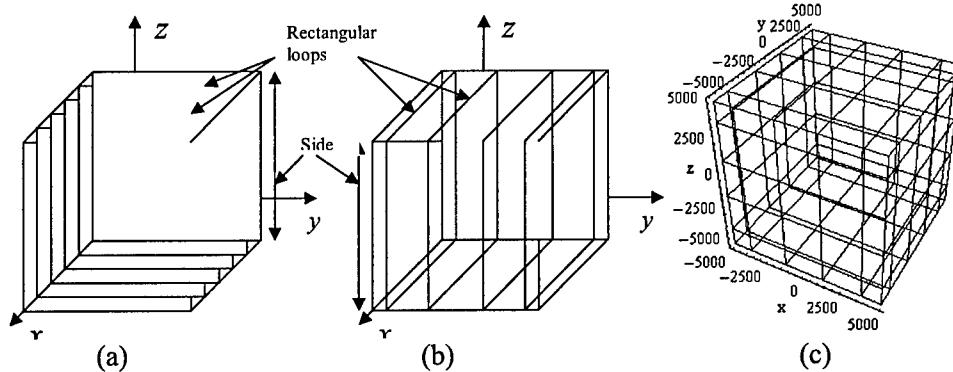


Figure 7 (a, b, c). A cubical precipitate with a distribution of rectangular dislocation loops (four each) along (a)  $x$ -axis and (b)  $y$ -axis, representing the misfit (normal eigenstrain) along these axes respectively, (c) A mesh of loops is generated along all three axes.

One of the main advantages of this distributed-dislocation method is that it can easily handle particles with difficult shapes. For example some real gamma prima particles are not exact cubes but rather cuboidal in shape where there have truncated corners similar to Figure 8. Loops can be distributed in this volume in all three perpendicular directions to produce a dilatation. Moreover, the method easily allows for a non-uniform distribution of eigenstrains by simply distributing the loops in a non-uniform fashion along any direction. This feature is valuable when considering the anisotropy of dilatation. Finally, although not shown here, the method is equally applicable to shear eigenstrains. Figure 9 shows a typical stress result for a perfect cubical particle calculated from its center out, along the y-axis in this case. The y-axis here happens to intersect the center of one of the cube faces at a distance of 5000 units.

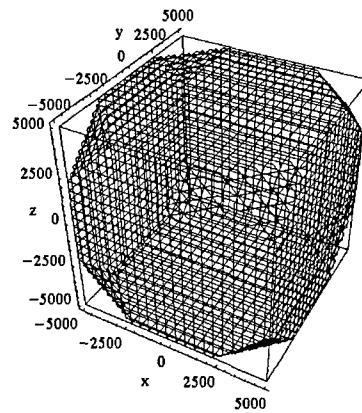


Figure 8. A cuboidal precipitate (20×20×20 loop mesh) with uniform chamfer at the corners. The chamfer cut length is uniform and is 25% of the total face-to-face distance (i.e. edge length of an enclosing cube). These cuboidal shapes are emulated at the corners using octagonal loops. Square loops are used in between corners as in the case of perfect cube.

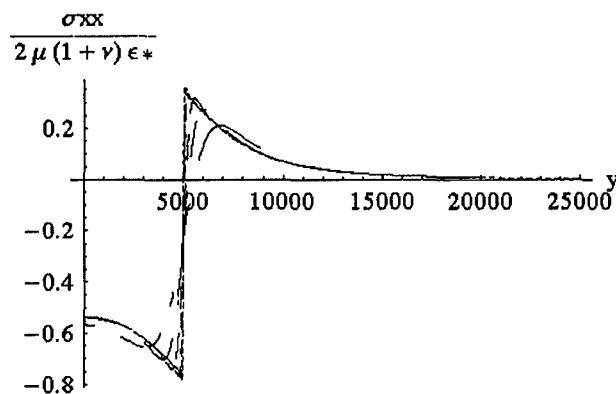


Figure 9. Normalized  $\sigma_{xx}$  plotted along y-direction for  $\varepsilon_{xx}^* = \varepsilon_{yy}^* = \varepsilon_{zz}^* = 0$ .

## Modeling Free Surface Effects in 3-D DD

The objective of this part of the research is to try and quantify the effect of free surfaces on the plasticity, e.g. flow stress, of a material within the context of 3-D DD. The DD computational cell is typically cubic or parallelepiped in shape. The surfaces of such shape are typically free surfaces. The fundamental stress solution used for dislocations in the cell is based on an infinite medium. This solution creates unphysical tractions on the free surfaces. We developed a method by which we enforce a physical zero traction condition on select or collocation points on the surface. Such points are shown in Figure 10 as the centers of square or rectangles on a surface  $S$ . A dislocation segment like  $A_1B_1$  would produce unphysical tractions at these points. If one assumes that each rectangle or square is a stress-producing dislocation loop then our goal is to find the Burgers vector of these mathematical loops such that zero traction is enforced at the collocation points. The more collocation points the better (see Figure 11). Such a stated requirement translates into a system of linear algebraic equations that is to be solved for the unknown Burgers vector components. Once the Burgers vectors of the loops are determined then the “image stresses” or free surface effect is simply that produced by the surface loops onto the dislocation segment  $A_1B_1$  (Yan et al. 2003, 2004). As part of the method, the stress field of a dislocation loop, as shown in the inset of Figure 10, had to be developed. Treating all surfaces of a computational cell with this method in the DD code, the stress-strain diagrams of a material subject to a constant strain rate is shown in Figure 11. The figure shows an effect on the flow stress of about 15% for the particular choice of parameters or problem considered. Other situations might produce a smaller or larger effect.

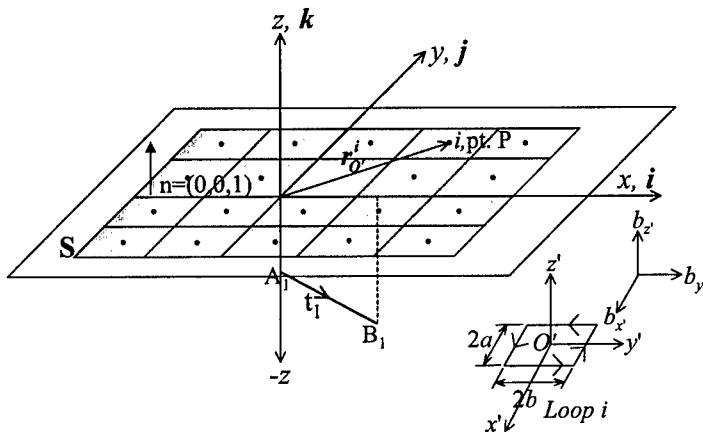


Figure 10. Segment  $A_1B_1$  beneath a free surface. Also, a mesh of rectangular elements, representing generally-prismatic dislocation loops, covering area  $S$  upon which stress traction annulment is sought. The inset shows one of these loops. The elements' centers are collocation points for the problem at hand. *Loop  $i$*  is centered at  $(x_{O'}^i, y_{O'}^i)$  with  $z_{O'}^i = 0$  in this case.

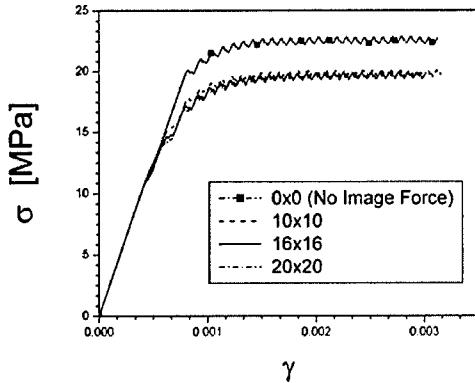
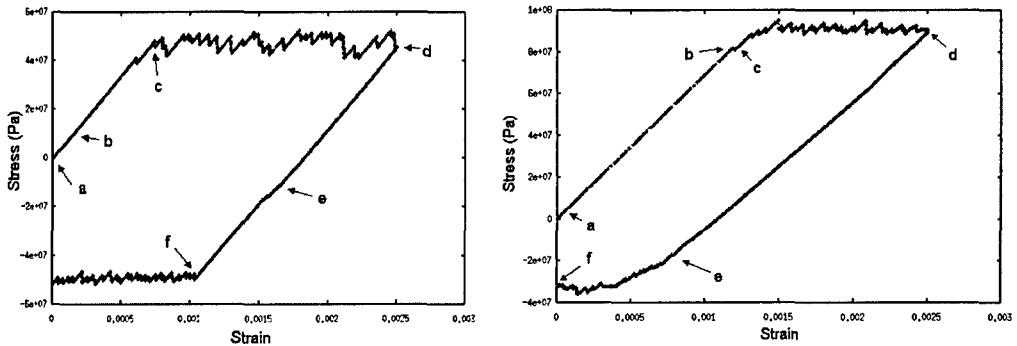


Figure 11. Stress-strain diagrams from DD simulations for one operational Frank-Read source in a cubic cell that is  $10,000b$  in side length. The source is close to the cell's center away from its surfaces. The line with a square symbol corresponds to no treatment of the traction-free boundary condition, and the other lines correspond to an external surface mesh density of  $10 \times 10$  loops,  $16 \times 16$  loops, and  $20 \times 20$  loops.

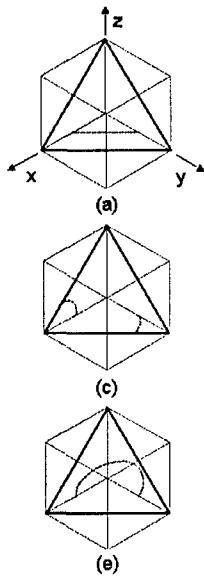
### Dislocation Dynamics (DD) Simulations of Cyclic Loading

The same methodology for studying the dislocation-particle interaction, described above, was used to simulate the uniaxial cyclic loading. The attention is to investigate the Bauschinger-like effect, or “strength differential,” in metals containing inclusion particles, although the slip plane considered in this study does not intersect the spherical particle in the model. The physical rationale is that the elastic interaction considered here actually occurs much more frequently in materials with dilute particle concentrations than the commonly conceived Orowan looping events. This is because a given dislocation segment is expected to traverse the metal matrix for a relatively long distance before, if ever, approaching a particle head-on.

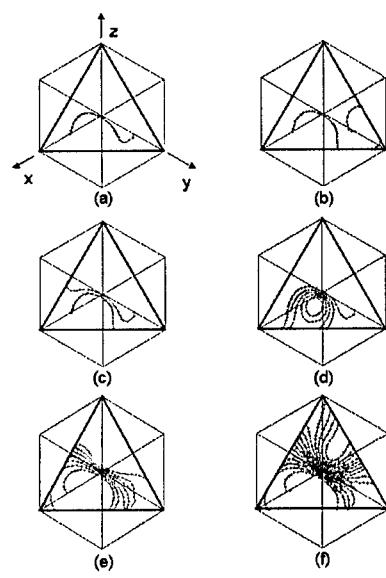
Figure 12(a) shows the simulated overall uniaxial stress-strain response of the crystal with no embedded particle. The simulation features a forward tensile loading to an applied strain of 0.0025, followed by a reversed loading back to zero strain. It is clear that this reference case shows no strength differential. Figure 12(b) shows the simulated stress-strain response of the crystal containing a spherical particle of radius  $2,000 b$  ( $b$  is the magnitude of a Burgers vector). The closest distance between the slip plane and the edge of the particle is  $887 b$ . The existence of the elastic misfit field causes a strong strength differential: the magnitude of tensile flow stress is significantly greater than that of the compression. The reasons behind this Bauschinger-like effect can be seen by examining the evolution of dislocation configurations obtained from the present DD simulations. Examples are shown in Figures 13 and 14, which demonstrate the dislocation sub-structure in the models without and with, respectively, a misfit particle. The “back stress” concept can be employed to analyze the simulation result. The effects of particle size and applied strain rate on the overall cyclic material behavior are also studied (Leger et al. 2004).



**Figure 12.** Simulated stress-strain curves during loading and unloading for the models (a) without and (b) with a misfit spherical particle.



**Figure 13.** Dislocation configurations corresponding to points labeled on the simulated stress-strain diagram in Figure 1(a) of the crystal with no embedded particle.

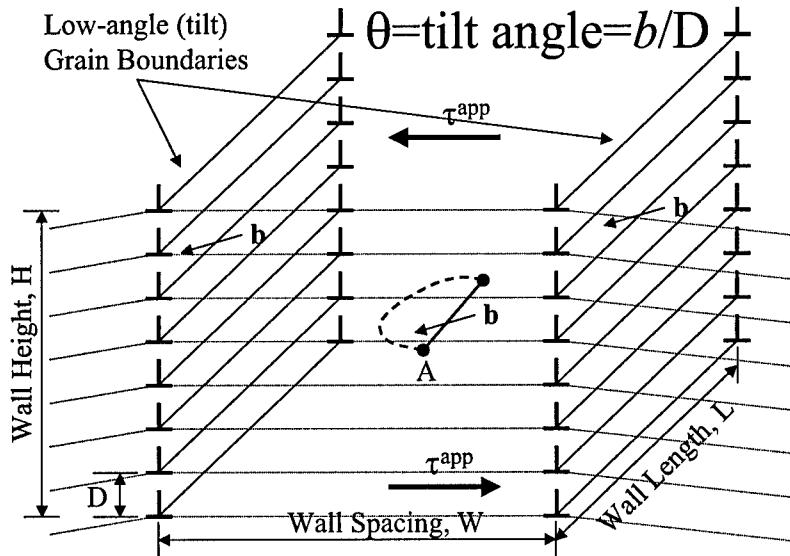


**Figure 14.** Dislocation configurations corresponding to points labeled on the simulated stress-strain diagram in Figure 1(b) of the crystal with an embedded particle.

### Simulations of Dislocation-Grain Boundary Interaction

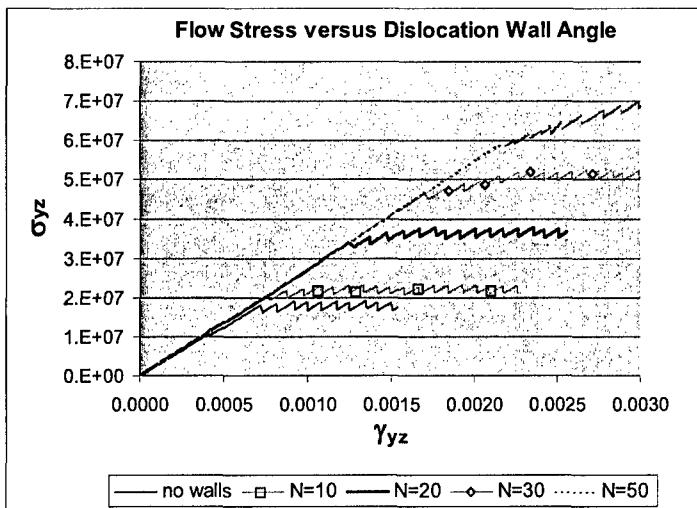
We have performed some preliminary simulations of the interaction between gliding dislocations and tilt walls or low-angle grain boundaries in an aluminum matrix. Several interesting results came out of this work. Figure 15 shows the parameters of pertinence to the

simulations, i.e. the problem set-up which is a dislocation source between two walls of the same tilt angle.

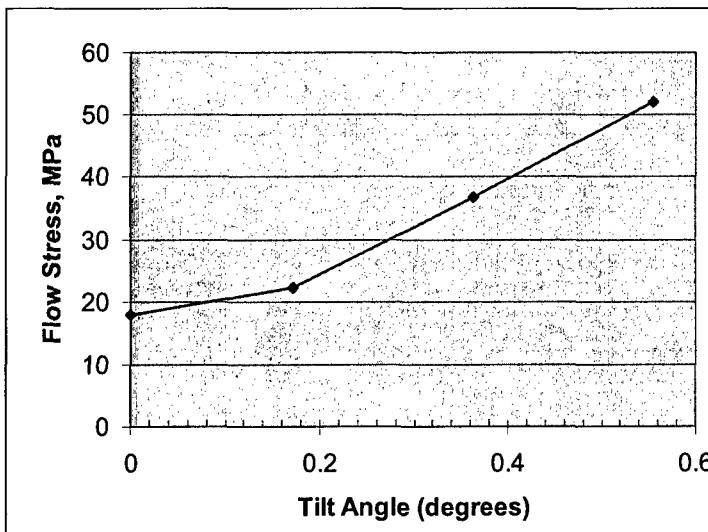


**Figure 15.** A schematic of two low-angle grain boundaries or tilt walls separated by a distance  $W$ . The walls have the same Burgers vector  $b$  as dislocation source  $A$  which is pinned at both ends. Dislocation  $A$  is free to glide under applied stress  $\tau^{\text{app}}$  and the stress field of the walls. The walls have the same sign.

The impedance to dislocation motion offered by the tilt walls manifests itself in a higher flow stress value on a stress-strain curve. Fixing the wall spacing, height and length, the number of dislocations within a wall (or equivalently the spacing of wall dislocations or tilt angle) can be varied to study their effect on the flow stress. Figure 16 shows the results of such a study. In this figure, it is clearly observed that as the number of wall dislocations  $N$  increased the flow stress value for the material increased. If one uses this figure to plot flow stress versus the tilt angle, one obtains the curve in Figure 17 where a zero tilt angle corresponds to the case of no walls present (i.e. an infinite spacing between the wall dislocations). The curve shows a non-linear dependence of flow stress on the tilt angle. It is important here to note that this hardening effect in the material is *not* a Hall-Petch effect. In other words, we are not measuring here the dependence of the flow stress on the cell size, i.e. the wall spacing. Instead, flow stress is demonstrated to be a function of the tilt angle, something that has not been focused on in previous studies.



**Figure 16.** The effect of the number of dislocations within a wall of fixed  $H$  (or equivalently the spacing of wall dislocations or tilt angle) on the flow stress of the material.



**Figure 17.** The flow stress versus the dislocation tilt wall angle (based on Figure 5).

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Tariq Khraishi	Assistant Professor, University of New Mexico
Yu-Lin Shen	Associate Professor, University of New Mexico

## Publications

1. Lerma, J., Khraishi, T., Shen, Y.-L., Wirth, B. D., 2003, "The Elastic Fields of Misfit Cylindrical Particles: A Dislocation-Based Numerical Approach," *Mechanics Research Communications*, Vol. 30, Issue 4, pp. 325-334.
2. Yan, L., Khraishi, T. A., Shen, Y.-L., Horstemeyer, M. F., 2003, "A Numerical Method for the Treatment of Image Stresses in Dislocation Dynamics Simulations," Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics, K. J. Bathe (editor), pp. 776-779.
3. Khraishi, T. A., Yan, L., Shen, Y.-L., 2003, "Modelling Strengthening Mechanisms in Solids Using Dislocation Dynamics," Proceedings of the ASME International Mechanical Engineering Congress and Exposition (IMECE'03), Washington, D.C., Nov. 16-21, Materials Division (MD), Vol. 98, pp. 263-271.
4. Lerma, J., Khraishi, T., Shen, Y.-L., Wirth, B. D., 2003, "A Distributed-Dislocation Method for Generalized Eigenstrain Problems", Proceedings of the First International Conference on Computational Methods in Materials Characterisation 2003, A. A. Mammoli and C. A. Brebbia (editors), pp. 185-194.
5. Khraishi, T. A., Yan, L., Shen, Y.-L., 2004, "Dynamic Simulations of the Interaction between Dislocations and Dilute Particle Concentrations in Metal-Matrix Composites (MMCs)," *International Journal of Plasticity*, Vol. 20, issue 6, pp. 1039-1057.
6. Leger, R. W., Khraishi, T. A. and Shen, Y.-L., 2004, "A Dislocation Dynamics Study of Strength Differential in Particle-Containing Metals during Cyclic Loading," *Journal of Materials Science*, Vol. 39, no. 11, pp. 3593-3604.
7. Yan, L., Khraishi, T. A., Shen, Y.-L., Horstemeyer, M. F., 2004, "A Distributed-Dislocation Method for Treating Free-Surface Image Stresses in 3D Dislocation

Dynamics Simulations," *Modelling and Simulation in Materials Science and Engineering*, Vol. 12, no. 4, pp. S289-S301.

8. Leger, R. W., Shen, Y.-L., Khraishi, T. A., 2004, "Defect Nucleation during Nanoindentation: An Atomistic Analysis," *Journal of Computational and Theoretical Nanoscience*, Vol. 1, no. 3, pp. 259-262.
9. Marina Popova, Yu-Lin Shen, Tariq A. Khraishi, 2005, "Atomistic Simulation of Dislocation Interactions in a Model Crystal Subjected to Shear," *Molecular Simulation*, Vol. 31, nos. 14-15, pp. 1043-1049.

#### **Awards Received**

ASME Fellow—awarded to Yu-Lin Shen in May 2005

ANS (American Nuclear Society) 2004 Materials Science and Technology Division Literary Award. Paper titled: "Mechanical Property Degradation in Irradiated Materials: A Multiscale Modeling Approach" in *Nuclear Instruments and Methods B*. Work co-authored by Tariq Khraishi and others.

ASME Graduate Teaching Fellowship-awarded to Jesus Lerma in November 2004.